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United States Environmental Protection Agency
Washington, DC 20460

E. White

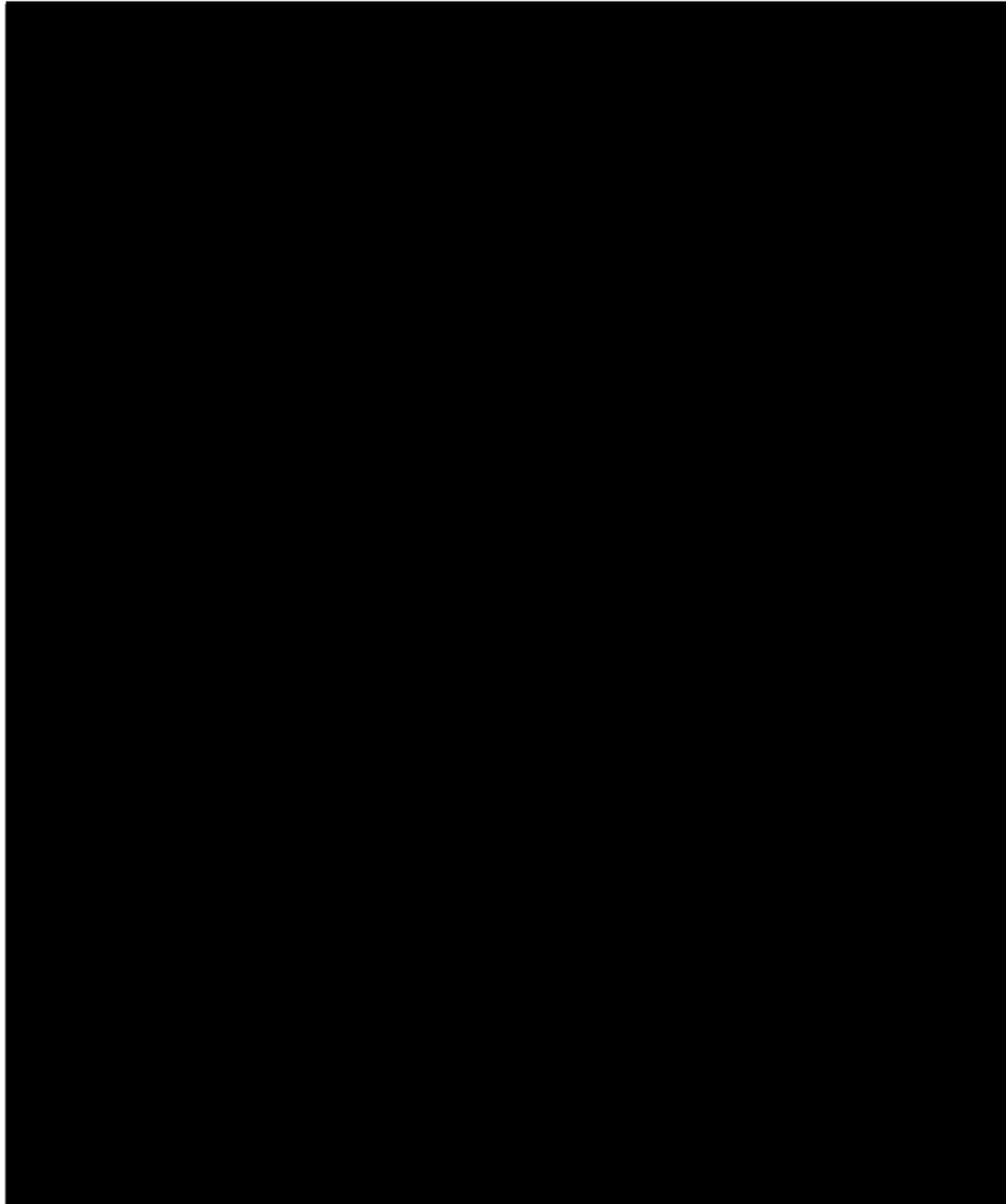
ORIGINAL

Document Description

SAT L-07-291

Date

7/20/07



STRUCTURE ACTIVITY TEAM REPORT ver. 04/98

Case #: L-07-0291

DCN:

SAT Date: 6/29/2007

SAT Chair: V. Nabholz

Submitter: Tracerco

Chemical Name:

Benzoic acid, 4-fluoro-, sodium salt (1:1)

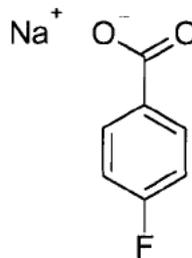
CAS RN:

499-90-1

Trade Name:

Tracerco 140

Structure



Molecular Formula:

$C_7H_4FNaO_2$

Molecular Wt. 162

WT%<500:

WT%<1000:

MP:

BP:

>500

Eq. Wt:

H2O Sol (g/L):

>100

V.P.

<0.000001

Max. Prod. Volume (kg/yr):

1000

Physical State:

Solid

USE:

Tracer chemical to measure flow in deep oil-bearing strata. Concurrently submitted similar cases L-07-290 to L-07-295.

Analog L-07-271 has this same use. There are 35 reference in file CA on STN, none for this use.

P2REC: CRSS: forward. P2 Claim: The LVE substance is a substitute for radionuclide tracers to measure the flow rate in oil-bearing strata. The LVE substance has been awarded Offshore Chemical Notification System Gold Band Status by European regulatory authorities.

Related Case Numbers	Case Role	Related Case Numbers	Case Role

Focus

Date: JUL 9 2007

Results:

Conditional Grant P2REC →



STRUCTURE ACTIVITY TEAM REPORT 29 June 2007

CASE NUMBERS: L07-0290 to L07-~~0330~~³⁰⁰

L07-0290 (F2)
L07-0291 (F)
L07-0292 (F2)
L07-0293 (F2)
L07-0294 (F2)
L07-0295 (F2)
L07-0296 (F4)
L07-0297 (F3)
L07-0298 (CF3)
L07-0299 (CF3)
L07-0300 (CF3)

P2REC: substitute for radionuclide tracers

RELATED CASES:

L07-0271 (F)



CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN: HEALTH ECOTOX

LEVEL: 1-2 1

KEYWORDS: DEVEL, LIVER, KIDNEY, SENS-ASTHMA, MUTA

SUMMARY OF ASSESSMENT:

FATE: MW162 to 216
solids with mp for L070271 (F) = 126 °C (M)
log Kow for the free acid = 1.8 to 2.9 (ClogP), 1.2 to 2.8 (EPI),
1.59 to 3.10 (M)
log Kow for L070271 = -5.87 with pH? (HPLC)
log Kow for L070296 = -2.11 with pH? (HPLC)
log Kow for L070297 = -3.62 with pH? (HPLC)
log Kow for L070298 = -1.64 with pH? (HPLC)
S > 200 mg/L to > 10 g/L at 20 °C (P)
vp < 1.0E-6 mm Hg or torr at 25 °C (P)
bp = 460 °C (P)
H for the covalent ion pair = 1.2E-7 to 9.5E-7 (P)
log Koc for the covalent ion pair = 1.4 to 2.0 (P)
log fish BCF = 0.50 (P)
sorption to sludge = low (P)

test data for L070271 for aerobic biodegradation in seawater at 20 C, via closed bottle (OECD306) were:

time (d)	biodegradation (percent)
5	0
14	2
28	63

test data for aerobic biodegradation for the [REDACTED] of L070299 from [REDACTED] were:
15% biodegradation in 28 d, thus, not readily biodegradable via CO2 evolution in modified Sturm test (OECD301B); if test result is due solely to ester hydrolysis and degradation of the [REDACTED] moiety, then removal via POTW of the parent would be $\geq 90\%$ but notifier did not measure degradation products;

POTW removal = 0% to 90 via sorption and possible biodegradation
time for complete ultimate aerobic biodegradation = weeks to => months

sorption to soils and sediments = low (P)

PBT Potential: P2B1T2 to P3B1T2

*CEB FATE: migration to ground water = rapid

HEALTH: Absorption nil thru skin based on physical/chemical properties; good thru lungs based on analogs; and good thru the GI tract based on analogs;

test data for the [REDACTED] [REDACTED] of L070299, [REDACTED], were:

rat acute oral LD50 = 800 mg/kg with toxic signs; LD100 = 2 g/kg, LD0 = 300 mg/kg;

rat acute dermal LD0 = 2.0 g/kg with no toxic signs;

slight and transient (2 d) skin irritation in rabbits;

slight and transient (1 d) eye irritation in rabbits;

Ames test was negative;

E. coli test was negative;

chromosome aberration test with V79 cells was positive with activation, but negative without activation;

no skin sensitization in guinea pigs (M&K);

rat 28-d subchronic oral-gavage with doses = 1000, 300, and 100 mg/kg/d with NOAEL = 100 mg/kg/d and LOEL = 300 mg/kg/d based on salivation and increased water consumption; effects at 1000 mg/kg/d were slight to severe salivation, unsteady gait, motor activity significantly decreased and effects to the liver and kidneys;

concern for asthma and developmental toxicity based on data for benzoic acid, note: the mechanism for the asthma is unknown;

concern for possible mutagenicity, liver toxicity, and kidney toxicity based on data for [REDACTED] which was the [REDACTED] [REDACTED] of L070299, however, the [REDACTED] will have some acylating activity

which is absent in the acid, thus, the acid will be less toxic than the [REDACTED];

low to moderate concern for toxicity

*CEB HEALTH: Exposures to humans: inhalation, ingestion, and drinking water;

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50	>	100.0	P
SW fish 96-h LC50	=	440.0	M S,N L070271
SW fish 96-h LC50	>	320.0	M S,N L070290
SW fish 96-h LC50	>	320.0	M S,N L070291
daphnid 48-h LC50	>	100.0	P
SW invert Ac ton 48-h LC50	=	2830.0	M S,N L070271
SW invert Ac ton 48-h LC50	=	1500.0	M S,N L070290
SW invert Ac ton 48-h LC50	=	430.0	M S,N L070291
SW invert Ac ton 48-h LC50	=	480.0	M S,N L070292
SW invert Ac ton 48-h LC50	=	270.0	M S,N L070293
SW invert Ac ton 48-h LC50	=	250.0	M S,N L070294
SW invert Ac ton 48-h LC50	=	250.0	M S,N L070295
SW invert Ac ton 48-h LC50	=	300.0	M S,N L070296
SW invert Ac ton 48-h LC50	=	430.0	M S,N L070297
SW invert Ac ton 48-h LC50	=	440.0	M S,N L070298
SW invert Ac ton 48-h LC50	=	170.0	M S,N L070299
SW invert Ac ton 48-h LC50	=	130.0	M S,N L070300
green algal 96-h EC50	>	100.0	P
SW algae Sk cost 72-h EC50 c	=	250.0	M S,N L070271
SW algae Sk cost 72-h EC50 r	>	10000.0	M S,N L070290
SW algae Sk cost 72-h EC50 r	=	430.0	M S,N L070291
SW algae Sk cost 72-h EC50 r	=	660.0	M S,N L070292
SW algae Sk cost 72-h EC50 r	=	2100.0	M S,N L070296
SW algae Sk cost 72-h EC50 r	=	1500.0	M S,N L070297
SW algae Sk cost 72-h EC50 r	=	700.0	M S,N L070300
fish chronic value	>	10.0	P
daphnid ChV	>	10.0	P
algal ChV	>	10.0	P
SW algae Sk cost ChV c	=	100.0	M S,N L070271
SW algae Sk cost ChV r	=	5600.0	M S,N L070290
SW algae Sk cost ChV r	<	100.0	M S,N L070291
SW algae Sk cost ChV r	=	320.0	M S,N L070292
SW algae Sk cost ChV r	=	1000.0	M S,N L070296
SW algae Sk cost ChV r	=	320.0	M S,N L070297
SW algae Sk cost ChV r	=	320.0	M S,N L070300
benthic			
SW invert Coror vol 10-d LC50	=	6558.0	mg/kg DWT M S,N L070271
SW invert Coror vol 10-d NOEC	=	470.0	mg/kg DWT M S,N L070271
SW invert Coror vol 10-d LC50	=	7300.0	mg/kg DWT M S,N L070290
SW invert Coror vol 10-d NOEC	=	1400.0	mg/kg DWT M S,N L070290
SW invert Coror vol 10-d LC50	=	3800.0	mg/kg DWT M S,N L070291
SW invert Coror vol 10-d NOEC	=	150.0	mg/kg DWT M S,N L070291

SW invert Coror vol 10-d LC50	=	6700.0	mg/kg	DWT M S,N	L070292
SW invert Coror vol 10-d NOEC	=	1400.0	mg/kg	DWT M S,N	L070292
SW invert Coror vol 10-d LC50	=	410.0	mg/kg	DWT M S,N	L070296
SW invert Coror vol 10-d NOEC	=	130.0	mg/kg	DWT M S,N	L070296
SW invert Coror vol 10-d LC50	=	330.0	mg/kg	DWT M S,N	L070297
SW invert Coror vol 10-d NOEC	=	160.0	mg/kg	DWT M S,N	L070297
SW invert Coror vol 10-d LC50	=	280.0	mg/kg	DWT M S,N	L070300
SW invert Coror vol 10-d NOEC	=	16.0	mg/kg	DWT M S,N	L070300

Predictions are based on SARs for neutral organic chemicals with 10X less toxicity due to the substitution of the acid, or SARs for anionic surfactants-carboxylic acid-C4.Na; SAR chemical class = surfactant-anionic-F1 to F4 and CF3 benzene-COO.Na; MW162 to 216; solids with mp for L070271 (F) = 126 °C (M); log Kow for the free acid = 1.8 to 2.9 (ClogP), 1.2 to 2.8 (EPI), 1.59 to 3.10 (M); log Kow for L070271 = -5.87 with pH? (HPLC); S > 200 mg/L at 20 °C (P); pH7; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L; low concern for toxicity assessment factor = 10.0 concern concentration = 1.0 mg/L (ppm) *CEB ECOTOX: No releases to water;

P2REC: forward to FOCUS with support.

SAT Co-chair: Vince Nabholz, 564.8909.

GTOX Report

PMN No.
L-07-0291

CAS No.
000499-90-1

Rcvd:
06/18/07

OECD
Incomplet

ID: Rec# 4 : 855

S/A
S

Name of Analog

Reviewer
ked

with activation

without activation

Positive Strains

Salmonella Assay:

CHO:

Chromosomal Aberration

CHL:

V79:

E. coli Reverse Mutation:

Mouse Micronucleus Assay:

Route:

Rat Hepatocytes Unscheduled DNA Synthesis:

Other GTOX Results

Comments

ECOTOX:

Fate:

WS/Log P:

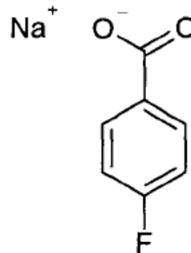
LogP=-0.1, p.27

NCSAB SAT REPORT

PMN: L-07-0291 CAS RN: 499-90-

Chemical Name: Benzoic acid, 4-fluoro-, sodium salt (1:1)
 Analogs:
 Production Volume: 1000.0t

Structure:

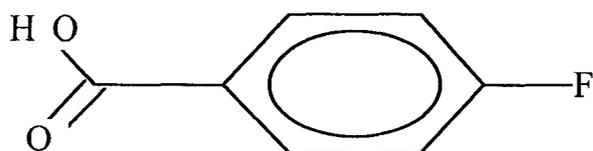


Use: Use as a tracer chemical to measure flow in deep oil-bearing strata. Concurrently submitted similar cases L-07-290 to L-07-295. Analog L-07-271 has this same use. There are 35 reference in file CA on STN, none for this use. P2REC: CRSS: forward. P2 Claim: The LVE substance is a substitute for radionuclide tracers to measure the flow rate in oil-bearing strata. The LVE substance has been awarded Offshore Chemical Notification System Gold.

Formula: $C_7H_4FNaO_2$ Eq Wt:
 Mol Weight: 162.10 Wt%<500: Wt%<1000
 MP: BP: >500 VP: <0.000001
 H2O Sol (g/L): >100 Physical State: Solid Log P:

Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h			
Daphnid 48-h			
Algal 96-h			
Fish ChV			
Daphnid ChV			
Algal ChV			
BCF			

CHEMICAL CLASS: SAR:
 ECOTOX CONCERN H M L CONCERN CONCENTRATION
 DATE ASSESSOR:



SMILES : Fc1ccc(cc1)C(=O)O
 CHEM :
 CAS Num:
 ChemID1:
 ChemID2:
 ChemID3:
 MOL FOR: C7 H5 F1 O2
 MOL WT : 140.11
 Log Kow: 2.13 (User entered)
 Melt Pt: 187.00 deg C
 Wat Sol: 47.01 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

 Neutral Organics-acid

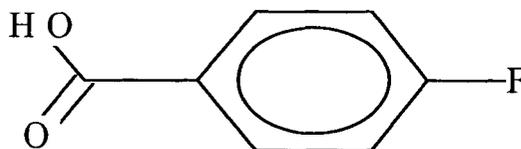
ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	144.962 *

--> Acid moiety found: Predicted values multiplied by 10

Neutral Organics-acid	: Fish	96-hr	LC50	783.943 *
Neutral Organics-acid	: Fish	14-day	LC50	1449.620 *
Neutral Organics-acid	: Daphnid	48-hr	LC50	847.587 *
Neutral Organics-acid	: Green Algae	96-hr	EC50	533.868 *
Neutral Organics-acid	: Fish	30-day	ChV	103.130 *
Neutral Organics-acid	: Daphnid	16-day	EC50	46.013
Neutral Organics-acid	: Green Algae	96-hr	ChV	57.553 *
Neutral Organics-acid	: Fish (SW)	96-hr	LC50	191.242 *
Neutral Organics-acid	: Mysid Shrimp	96-hr	LC50	206.056 *

ECOSAR Class	Organism	Duration	End Pt	mg/kg (ppm) dry wt soil
Neutral Organics-acid	: Earthworm	14-day	LC50	7860.393 *

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.
 Fish and daphnid acute toxicity log Kow cutoff: 5.0
 Green algal EC50 toxicity log Kow cutoff: 6.4
 Chronic toxicity log Kow cutoff: 8.0
 MW cutoff: 1000



SMILES : Fc1ccc(cc1)C(=O)O
 CHEM :
 MOL FOR: C7 H5 F1 O2
 MOL WT : 140.11

----- EPI SUMMARY (v3.12) -----

Physical Property Inputs:

Water Solubility (mg/L):	-----	Log Kow (oct-water):	2.13
Vapor Pressure (mm Hg):	-----	Boiling Pt (deg C):	-----
Henry LC (atm-m3/mole):	-----	Melting Pt (deg C):	187.00

Log Kow (KOWWIN v1.67 estimate) = 2.07 Exp database: 2.07

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):

Boiling Pt (deg C):	245.45		
Melting Pt (deg C):	51.64	MP(exp database):	185 deg C
VP(mm Hg,25 deg C):	0.00068		

Water Solubility estimate (WSKOW v1.41): 578.5 mg/L

Water Solubility estimate (fragments): 1485.9 mg/L

Henrys Law Constant (atm-m3/mole) [HENRYWIN v3.10]:

Bond Method:	1.27E-007	Group Method:	1.28E-007
Henrys LC [VP/WSol estimate using EPI values]:	2.167E-007 atm-m3/mole		

Biodegradation Estimates (BIOWIN v4.02):

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:

OH Half-Life = 7.509 Days (12-hr day; 1.5E6 OH/cm3)
 No Ozone Reaction Estimation

Soil Adsorption (PCKOCWIN v1.66): Koc = 23.47 Log Koc = 1.371

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Rate constants can NOT be estimated for this structure!

BCF estimate (BCFWIN v2.15): Log BCF = 0.500 (BCF = 3.162)

Volatilization from Water: (Henry LC = 1.28e-007 atm-m3/mole)

Half-Lives: Model River = 5415 hr, Model Lake = 5.918e+004 hr

Removal In Wastewater Treatment (percents, 99% recommended maximum):

TOTAL: 2.39, Biodeg: 0.10, Sludge: 2.29, Air: 0.01

Level III Fugacity Model (conc %, half-life hr):

Air(0.835%,180), Water(23.1%,900), Soil(76%,1.8e+003), Sediment(0.105%,8.1e+003)
 Persistence Time: 1.22e+003 hr

CHEMICAL: Unknown

10:31:19 06/27/:7

MOL WT : 140.12

MOL FOR: C7H5F1O2

SMILES : Fc1ccc(cc1)C(O)=O

ISOC-ID: -a-aaa-aa-

FRAG-ID: 1 2 2 2

H-COUNT: 11 11 1

Class	Type	Contribution Description	Comment	Value
FRAGMENT	# 1	Fluoride	MEASURED	0.370
FRAGMENT	# 2	Carboxy (ZW-)	MEASURED	-0.030
ISOLATING	CARBON	6 Aromatic isolating carbon(s)		0.780
EXFRAGMENT	HYDROG	4 Hydrogen(s) on isolating carbons		0.908
ELECTRONIC	SIGRHO	1 Potential interactions; 1.00 used	withinRing	0.098
RESULT	v3.3	All fragments measured	ESTIMATE	2.126

ATTENDEES

SIGNATURE

CHEMISTRY

- Paul Bickart
- Diana Darling
- Rich Engler
- Greg Fritz
- Daniel Lin
- Kathy Schechter

Paul Bickart

Kathy Schechter

ENVIRONMENTAL FATE

- Bob Boethling
- Wen-Hsiung Lee
- Laurence Libelo
- David Lynch
- Andy Mamantov

HEALTH

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- Steve Cragg
- Leonard Keifer
- David Lai
- Jim Murphy
- Deborah Norris
- Ronald Ward
- Yin Tak Woo

Michael Cimino
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Leonard Keifer
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ENVIRONMENTAL EFFECTS

- Gordon Cash
- Vince Nabholz
- Maggie Wilson

Gordon Cash

SAT CHAIR/OTHER

- Rebecca Jones
- Leonard Keifer
- Vince Nabholz
- Jim Kwiat

Vince Nabholz